

Guide for Validation of Nuclear Criticality Safety Computational Methodology

Science Applications International Corporation

**U.S. Nuclear Regulatory Commission
Office of Nuclear Material Safety and Safeguards
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ABSTRACT

Evaluations for nuclear criticality safety must assure that subcritical conditions are present under both normal and credible off-normal conditions. Such evaluations typically rely upon computational techniques that are capable of modeling complex three-dimensional systems. An upper safety limit (USL) must be established based on a documented validation, under which acceptable calculated neutron multiplication or k_{eff} values must fall to be considered subcritical. The USL is established through the statistical evaluation of the calculational bias. The bias is the difference between critical experimental conditions similar to the area of applicability of interest and the calculated results of those experiments. This report describes procedures by which nuclear fuel cycle facility licensees may perform the validation activity, including determination of calculational bias, bias uncertainty, and an USL. Also included are suggested topics for inclusion in formal documentation of the validation activity.

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1. INTRODUCTION

Increasingly sophisticated tools are available to perform nuclear criticality safety (NCS) analyses. Most commonly the NCS analyses determine the conditions for subcriticality through the calculation of the neutron multiplication factor or k_{eff} of fissile systems. The calculational tools implement various techniques for solving the Boltzmann transport equation and determining the system k_{eff} . Experimentally derived data on neutron fission, scattering, and absorption cross sections are an essential component of the methodology for determining k_{eff} . These tools also may be used for determination of other critical parameters (e.g., critical mass), but for the purposes of this document it is assumed that the eigenvalue, k_{eff} , is the parameter to which the validation is directed.

1.1 NEED FOR VALIDATION METHODOLOGY GUIDANCE

For use in safety related analyses, the ability of a calculational methodology to accurately predict the subcriticality of a system must be well understood. The understanding of a calculational methodology's bias in predicting subcritical systems is obtained through the validation process. Validation includes identification of the difference between calculated and experimental results. This difference, called the bias, and the uncertainty associated with the bias are used in combination with additional subcritical margin to establish an upper safety limit (USL). Subcriticality is assured if calculated results are below the USL and are within the area of applicability for the validation.

This comparison of critical experiments and calculation is repeated for a variety of experiments so that inferences can be drawn through statistical analyses of the bias trends. It is necessary that a selection of experiments be relevant to the nature of the actual operation or analysis under evaluation. The range of experimental parameters used to validate the calculational methodology primarily defines the area(s) of applicability for the validation.

The statistical results from the bias trends are used to establish a safety limit. The calculational methodology includes the computer code implementing the physics and numerical techniques and the empirical data (cross sections) used in the calculation. Subsequent analyses, within the area of applicability, that predict a k_{eff} below the safety limit, after inclusion of associated calculational uncertainties, are expected to represent subcritical conditions.

This report describes procedures by which nuclear fuel cycle facility licensees may validate calculational techniques used for criticality safety analyses. These procedures are not the only means by which a criticality safety calculational methodology may be validated. The procedures described herein are compiled from existing validation practices within the industry and have been found to be straight forward and easily understandable. Use of these procedures can ensure that validations are performed and documented with sufficient rigor to demonstrate compliance with safety limits during facility operations.

In the sections that follow, each of the major procedural steps associated with code validation are discussed and citations are provided where other examples and details are available. Examples of selected procedural steps, including bias and bias uncertainty calculations and definition of the area of applicability are presented to assist in the application of the techniques.

1.2 RELATIONSHIP OF THE VALIDATION ACTIVITY TO SAFETY LIMITS AND THE NCS ANALYSIS PROGRAM

In order to establish an upper safety limit (USL) that reliably allows for determination of subcritical conditions, critical experiments (or near critical experiments) are compared to the calculated k_{eff} for those

experimental configurations. The validation activity, described herein, is directed to the computer program, supporting cross section libraries, and the hardware platform upon which the code system (program and data libraries) is implemented. An inexperienced user can also affect the bias through the modeling of critical experiments; therefore, it is essential that the modeling be performed by appropriately trained and qualified staff. Further discussion on sources of uncertainty in validation is found in NUREG/CR-5661.

The USL is represented by the following equation:

$$USL = 1.0 + Bias - \sigma_{Bias} - \Delta_{SM} - \Delta_{AOA} \quad (1)$$

Where the critical experiments are assumed to have a k_{eff} of unity, the bias is calculated as the difference between the calculated k_{eff} and the critical experiment modeled. Because a positive bias may be nonconservative, a bias is set to zero if the calculated average k_{eff} is greater than one. The statistical uncertainty in the bias is represented by σ_{Bias} and the subcritical margin is represented by Δ_{SM} . The term Δ_{AOA} is an additional subcritical margin to account for extensions in the area of applicability as discussed in Section 5 of this document. A value of zero is assigned to Δ_{AOA} if not extending the area of applicability.

In practice, the bias is determined as the difference between the average k_{eff} calculated from the statistical method and unity. The uncertainty in the bias is equated to some multiple of the uncertainty in the calculated k_{eff} 's.

The subcritical margin must be determined and justified based upon the reactivity worth and ability to control the parameter(s) and area(s) of applicability for the validation. For example, if a fissile container dimension has design tolerances of $\pm 1/2$ -inch and the evaluated reactivity or delta k_{eff} for a dimensional change of $1/2$ inch is 0.01, and such a change is clearly evident, then a margin of 0.02 would be justified. Margins of safety based on similar rationale have been documented in the literature (Winiarski and Risner, 1996).

Larger margins of safety must be established for areas of applicability beyond which there are critical experiments. An extrapolation of 5 to 10 percent of the parameter beyond the area of applicability would normally be considered large and would require an added subcritical margin. (Morey and Damon, 1999)

Safety limits for fissionable material operations are established for each fuel cycle licensee. It is required that the licensee's NCS program evaluate these operations for normal and credible abnormal operating conditions. The validation establishes a criterion, the USL, by which calculations of such anticipated or potential conditions may be assessed as being subcritical. These calculations are integral to the demonstration of compliance with operating safety limits in the license.

The following condition must be demonstrated for all normal and credible abnormal operating conditions:

$$k_{calc} + 2 \sigma_{calc} < USL \quad (2)$$

where:

k_{calc} is the calculated k_{eff} returned by the method and σ_{calc} is the uncertainty.

The term σ_{calc} is typically chosen to be the uncertainty associated with Monte Carlo calculations. For discrete ordinates calculations, sensitivity analyses might need to be performed about the convergence region or about other parameters to determine the uncertainty value.

The performance and documentation of the validation activity is but one part of the necessary elements in an NCS program. The ability of a program to determine and implement limits and controls for safe and efficient operations is dependent on having other essential elements. Those elements, in addition to validation, include:

- *Verification that the code system is correctly installed as received from the developer or distribution center.* It is typically the responsibility of the code developer to verify that the radiation transport physics and cross section treatment processes are correctly implemented in the code system. The user is responsible for following the software installation instructions and demonstrating that the supplied sample problems execute correctly.
- *Configuration control program for the software and hardware.* Changes to the criticality safety code will require reverification and validation. Significant changes to the hardware and other system software will require that the code system be reverified and may entail revalidation. Each site must establish criteria for when such changes merit analysis to determine if the validation could be impacted by the change. A periodic confirmation test should be performed to ascertain that the criticality safety code system is unchanged. Typically a small number of runs are made and the results are compared to a standard set of results.
- *Staff training and qualification.* Appropriately trained and qualified staff must perform the validation, particularly modeling of the critical experiments, and conducting the subsequent NCS evaluations. If a validated NCS computational methodology is incorrectly used, the desired subcritical margin may not be maintained. It is therefore essential that each site or facility establish and implement requirements for staff qualification and training.
- *Site procedures and guidelines.* In addition to requirements for staff training and qualification, verification, and validation, each site or facility should have guidelines for performing NCS evaluations. Such guidelines are necessary to have consistency in the means for performing calculations. These guidelines should be followed in the modeling of critical experiments for the validation activity. For example, the site should have a standard value for Avogadro's number and require consistent container dimensions, treatment of reflectors, density relationships for solutions, guidelines for interpretation of results, and composition of chemical compounds and common materials. Lack of such standards can cause problems in validation and in performance of NCS evaluations (Carter, 1985).

This document only addresses validation. Guidance for other essential elements is provided in ANSI/ANS-8 standards and elsewhere.

2. ELEMENTS OF THE VALIDATION ACTIVITY

The ANSI/ANS-8.1-1998 standard provides basic requirements for validation of a calculational method. While there are many calculational methods for determining the subcritical state of a system, the basic requirements for establishing validity apply to all. The bias of a code system (implemented computational methodology, cross section library, and computer hardware) is determined by correlating the results of critical and near-critical experiments with calculated results for those experiments. The common practice, and that assumed by this document, is for comparison of the calculated k_{eff} to a critical or near critical system. Other parameters and physical states may be used as the basis for determining the calculational bias.

The bias can vary over the area (or areas) of applicability for the calculational method. It is sometimes also necessary to extend the area of applicability beyond the range for which experimental conditions exist. The desired area of applicability is drawn from the span of conditions or parameters over which the facility or site operates. Such conditions include: types of fissile nuclides, U-235 enrichment, fuel and moderator compounds or density, and moderator to fuel ratio.

Computational techniques, such as Monte Carlo, cross section data, and critical experiments all have associated calculational or experimental uncertainties. These uncertainties all contribute to the uncertainty in the calculational bias. Allowances must be made for the bias and its uncertainty to ensure that calculated subcritical conditions are actually subcritical. Statistical techniques exist for evaluating the bias uncertainty and for establishing limits that can reliably be used to determine subcriticality. The highest calculated k_{eff} that can be used in establishing subcritical safety limits and operating controls is referred to as the upper safety limit (USL).

The validation activity must be documented in a formal manner. The validation report must contain sufficient detail, clarity, and specificity to allow independent duplication of the results. The experimental data and parameters derived from this data must be identified. The area of applicability for the validation must be stated. The bias, its uncertainty, and margin of subcriticality over the area of applicability must be stated. Additionally, the adequacy of the margin of subcriticality must be justified.

2.1 DEFINE OPERATION/PROCESS TO IDENTIFY RANGE OF PARAMETERS TO BE VALIDATED

Prior to the initiation of the validation activity, the operating conditions and parameters for which the validation is to apply must be identified. The fissile isotope, enrichment of fissile isotope, fuel density, fuel chemical form, types of neutron moderators and reflectors, range of moderator to fissile isotope, neutron absorbers, and physical configurations are among the parameters to specify. These parameters will come to define the area of applicability for the validation effort.

2.2 SELECT CRITICAL EXPERIMENT DATA

After the desired range of operating conditions and parameters are identified, then appropriate critical experiments can be selected for use in the validation. Over the years, many critical experiments have been performed and documented with varying degrees of quality. Care should be taken to distinguish critical benchmarks from critical experiments. Critical benchmarks are critical experiments that have been peer reviewed, have relatively detailed descriptions of relevant experimental conditions and, in general, can be repeatedly modeled with consistent results by qualified NCS specialists. In other words, all critical benchmarks are critical experiments, but not all critical experiments are critical benchmarks. Although critical benchmarks are preferred for use in validating calculational methodologies, there may

be some instances where only critical experiment data are available. Care should be taken to make appropriate allowances for the larger, and perhaps unspecified, uncertainties inherent with such data.

Perhaps the best source of critical benchmarks is found in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* from the Nuclear Energy Agency of the Organization for Economic Co-Operation and Development (OECD-NEA).

Current listings of critical experiments, along with instructions for obtaining a copy of the handbook, distributed on CD-ROM, may be found on the internet. The critical experiments described in this handbook have been found by the ANSI/ANS-8 Subcommittee for NCS to be rigorously peer reviewed and should be accepted as refereed. (American Nuclear Society, Minutes of Subcommittee 8, "Fissionable Materials Outside Reactors," Albuquerque, NM – May 7, 1998, John A. Schlessor, Secretary, Subcommittee 8.) The part of this handbook considered as being peer reviewed is the actual description of the critical experiments.

The handbook provides the results of calculations using several standardized criticality safety neutronics codes. The developers of the handbook determined that it would be useful for others using similar calculational methods and cross section data to have a basis for comparison. The users are cautioned that these calculations do not comprise a validation of codes or cross section data. Only a limited number of the numerous input options available in most codes were exercised in the sample calculations in the handbook. The input files for the sample problems for various computer programs are available so that users of the handbook can identify which options were used to obtain the reported results. It is the responsibility of the user to ensure that use of these input files for any other purpose is consistent with proper criticality safety practices.

Other sources of critical experimental data may be used. However, care should be taken to check the quality of the data in terms of completeness of the description, consistency of the results, and rigor of the documentation. An attempt should also be made to contact personnel involved with, or familiar with, the particular experimental data to obtain insight as to the suitability for use. This type of information should be documented as completely as possible in the validation report.

In general, the critical experiments selected for inclusion in the validation must be representative of the types of materials, conditions, and operating parameters found in the actual operations to be modeled using the calculational method. A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a method or establish validity of the method for a given material or condition, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results. Given the limitations of available critical experimental data, there will likely be occasions when there are insufficient critical experiments to support validation of specific materials, conditions, or range of parameters. In this case, the area of applicability of the validation must be extended using techniques such as those described in Section 5.

2.3 MODEL EXPERIMENTS

The computer code system implementing the desired computational methodology for which the validation is to apply must be identified, installed, and verified on the computer. The sequence of execution of code modules within the desired code package must be specified. The cross section library to be used must be specified. For example, a validation might be performed for the SCALE 4.4 code

package, with the CSAS25 module executing the BONAMI, NITAWL, and KENO V.a codes and the 44-group ENDF/B-V cross section library. The computer and major hardware should also be described. For example, the SCALE 4.4 code package is installed on a personal computer, serial xx-xxxx, model ABCD, running the XYZ operating system, having IJK features.

Once the computer code is selected for validation and installed and verified on the computer platform, the selected critical experiments are coded into the format required by the computer program. This coding is to be performed by a qualified individual experienced in performing such calculations. Depending on the type of calculational methodology being validated, it may be necessary and desirable to simplify the geometric model. For example, the bare metal critical assembly known as Godiva, may be modeled as a one-dimensional spherical system. Care should be taken to avoid over simplification as this could result in a nonrepresentative model of the critical experiment.

For specific critical experiments, the facility or site may choose to use input files generated elsewhere to expedite the validation process. The site has the responsibility for ensuring that input files and the options selected are appropriate for use. Regardless of the source of the input file, the site must have reviewed the description of each critical experiment and determined that the representation of the experiment, including simplifying assumptions and options, are consistent with the intended use. In other words, the site must assume ownership of the input file. Use of input files from other validation reports without cognizance of the critical experiment may cause misleading results.

Each critical experiment and resultant input file should be assigned a unique identification. Sensitivity analyses performed for a specific critical experiment should be assigned unique identification. The identifier should be associated with parameters of significance and the specific critical experiment.

2.4 ANALYZE THE DATA

The input files should be executed using the code system being validated to calculate the effective neutron multiplication factor for the selected critical experiments. The output from each evaluation should be carefully reviewed to ascertain that the run executed correctly and satisfied the convergence criteria¹. The k_{calc} and associated σ_{calc} values should be tabulated with other descriptive information (i.e., run identification, independent parameters, etc.).

2.4.1 Determination of Bias and Bias Uncertainty

The validation must use a statistical analysis to determine bias and bias uncertainty in the calculation of k_{eff} . Following are descriptions of an approach for this analysis. The approach involves determining a weighted mean that incorporates the uncertainty from both the measurement (σ_{exp}) and the calculation method (σ_{calc}). In some sources of critical experiments, an overall uncertainty in the measured critical parameters has been determined and presented. Where these experimental uncertainties are documented the values should be used. Where no documentation is located to substantiate an experimental uncertainty, engineering judgement should be used, based upon factors such as the typical uncertainties

¹ Each computational methodology has its own criteria that determines if a calculation has executed properly and the results can be regarded as reasonable given the input. Discrete ordinates methodologies use convergence criteria in the conventional sense for numerical analysis. Monte-Carlo methods typically provide equivalent information (e.g., k_{eff} by generation or generation skipped and statistics on the distribution of neutron histories that is analogous to a convergence). It is the responsibility of the individual using the computational methodology to be qualified in its use, including judging if the calculation has converged.

of similar experiments. Although this appears artificial, it is a more realistic assumption than assuming that there is no error associated with the measurements in the critical experiments. A combined error can then be determined (assuming that the two errors are orthogonal since one is derived from actual measurement errors and the other is a calculational error of the method) by applying the following equation:

$$\sigma_i = \sqrt{\sigma_{calc}^2 + \sigma_{exp}^2} \quad (3)$$

A weighted mean k_{eff} (\bar{k}_{eff}) is calculated by using the weighting factor $1/\sigma_i^2$. The use of this factor reduces the "weight" of data with high uncertainty. Within a set of data, the " i^{th} " member of that set is shown with a subscript " i ". Henceforth, unless otherwise specified, the uncertainty for an " i^{th} " k_{eff} is shown as σ_i and is taken to mean the combined calculational and experimental uncertainty, shown above as σ_i .

The weighted equation variables for the single-sided lower tolerance limit are presented below:

Variance about the mean

$$s^2 = \frac{\left(\frac{1}{n-1}\right) \sum \frac{1}{\sigma_i^2} (k_{eff,i} - \bar{k}_{eff})^2}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} \quad (4)$$

Average total uncertainty

$$\bar{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} \quad (5)$$

The weighted mean k_{eff} value

$$\bar{k}_{eff} = \frac{\sum \frac{1}{\sigma_i^2} k_{eff,i}}{\sum \frac{1}{\sigma_i^2}} \quad (6)$$

The square root of the pooled variance is:

$$S_P = \sqrt{s^2 + \bar{\sigma}^2} \quad (7)$$

where:

- s^2 = variance about the mean
- $\bar{\sigma}$ = average total uncertainty
- n = number of critical experiments used in the validation

The square root of this pooled variance (S_p) is used as the mean bias uncertainty when applying the single-sided tolerance limit methods discussed in the next section. Bias is determined by the relation:

$$\text{Bias} = \bar{k}_{eff} - 1 \quad \text{if } \bar{k}_{eff} \text{ is less than 1, otherwise Bias} = 0 \quad (8)$$

A positive bias may be non-conservative and the NRC has indicated that licensees would not be permitted to use a positive bias (Morey and Damon, 1999). Where the bias is found to be positive, an adjusted bias of zero is to be used.

It may be necessary to make an adjustment to the calculated k_{eff} if the critical experiment being modeled was at other than a critical state (i.e., slightly super or subcritical). This adjustment is done by normalizing the k_{calc} value to the experimental value. This normalization assumes that the inherent bias in the calculation is not affected by the normalization, which is valid for small differences in k_{eff} . Under no circumstances is the absolute value of the bias to be made smaller. To normalize k_{eff} , the following formula applies:

$$k_{norm} = k_{calc} / k_{exp} \quad (9)$$

The normalized k_{eff} values are to be used in the subsequent determination of the USL.

2.4.2 Identify Trends in Data, Including Discussion of Methods for Establishing Bias Trends

Trends are determined through the use of regression fits to the calculated results. In many instances a linear fit is sufficient to determine a trend in the bias. The use of weighted or unweighted least squares is a means for determining the fit of a function. In the equations below, "x" is the independent variable representing some parameter (e.g., H/U-235). The variable "y" represents k_{eff} . Variables "a" and "b" are coefficients for the function. An example illustrating the fit of a straight line to a set of data is provided in Section 3.

The equations used to produce a weighted fit of a straight line to a set of data are given below.

$$Y(x) = a + bx \quad (10)$$

$$a = \frac{1}{\Delta} \left(\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} \right) \quad (11)$$

$$b = \frac{1}{\Delta} \left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} \right) \quad (12)$$

$$\Delta = \sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2 \quad (13)$$

There are many functions in addition to a straight line to which data can be fitted. Details on fitting functions to data are found in the literature. Extreme care must be exercised when fitting linear or non-linear functions to assure oneself that perceived relationships of nuclear parameters are real.

Goodness of Fit

There are two steps that should be employed when determining the goodness of fit. The first is to plot the data against the independent variable using different scales of axes. This allows for a visual evaluation on the effectiveness of the regression fit.

The second step is to numerically determine a goodness of fit after linear or non-linear relations are fit to the data. This adds a useful measure because visual inspection of the data plot and the associated fit will not necessarily reveal how good the fit is to the data. The linear correlation coefficient is one standard method used to numerically measure goodness of fit. The linear correlation coefficient is not the only, or possibly the best measure for goodness of fit. Another method is the χ^2 test, the details on this method are given in the literature.

The linear-correlation coefficient is a quantitative measure of the degree to which a linear relationship exists between two variables. For weighted data, the linear-correlation coefficient is

$$r = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\left[\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2 \right]} \sqrt{\left[\sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2 \right]}} \quad (14)$$

where the weighted mean for the independent parameter is

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} \quad \text{and} \quad \bar{y} = \bar{k}_{eff} \text{ from equation (6)} \quad (15)$$

The value of the linear-correlation coefficient is often expressed as a squared term, r^2 . The closer r^2 approaches the value of 1, the better the fit of the data to the linear equation.

Note that neither the linear correlation coefficient by itself, nor the comparison of coefficients can provide an absolute measure of how good the fit is.

2.4.3 Test for Normal or Other Distribution

The statistical evaluation performed must be appropriate for the assumed distribution of the data. There are numerous well-characterized distributions (i.e., Gaussian or normal, Student's t, Poisson, etc.) that can be demonstrated to be reasonable approximations to calculated k_{eff} values. For the purposes of this document, the normal distribution is used. If the data is normally distributed, then a technique such as a one-sided tolerance limit is used to determine the USL. If the data is not normally distributed, then a non-parametric analysis method must be used to determine the USL.

The literature describes several means of testing a hypothesis that data follow a normal distribution about some mean value. One such test, the Shapiro-Wilk test, is illustrated in Section 3 for a set of sample data.

Shapiro-Wilk Test for Normality

For cases where there are fewer than 50 samples, the Shapiro-Wilk Normality Test can be used to test the hypothesis that the calculated k_{eff} values are normally distributed about the mean k_{eff} . The calculations used in this determination are summarized by the following equations.

From Table A.5 a value for W can be obtained for the number of experiments. If W is less than the test statistic, W_p , then the data is considered normally distributed

where:

$$W_t = \frac{Y^2}{S^2} \quad (16)$$

$$Y = \sum_{j=1}^v \alpha_j (y_{(n+1-j)} - y_j) \quad (17)$$

$$S^2 = \sum (y_i - \bar{y})^2 = \sum (k_{eff_i} - \bar{k}_{eff})^2 \quad (18)$$

α_j \equiv Coefficients

y_i \equiv k_{eff} for critical experiment "i"

n \equiv Number of critical experiments

$$v = \frac{n}{2} \text{ for even } n, \frac{n-1}{2} \text{ for odd } n \quad (19)$$

Note: Computational results must be sorted in ascending order by k_{eff} for this test.

2.4.4 Select Statistical Method for Treatment of Data

The approach to establishing the USL relies on selection of an appropriate statistical treatment. This document presents a few of the common methods, but there are numerous treatments that can be used successfully. It is the responsibility of the facility or site performing the validation to justify the method selected. Three methods are discussed in this document. They are: the single-sided tolerance limit, single-sided tolerance band, and non-parametric methods where the k_{eff} values are not normally distributed about a mean value.

Single-Sided Tolerance Limit

A weighted single-sided lower tolerance limit (K_L) is a single lower limit above which a defined fraction of the true population of k_{eff} is expected to lie, with a prescribed confidence and within the area of applicability. The term "weighted" refers to a specific statistical technique where the uncertainties in the data are used to weight the data point. Data with high uncertainties will have less "weight" than data with small uncertainties.

A lower tolerance limit should be used when there are no trends apparent in the critical experiment results. Use of this limit requires the critical experiment results to have a normal statistical distribution (see Section 2.4.3). If the data does not have a normal statistical distribution, a non-parametric statistical treatment must be used.

Lower tolerance limits, at a minimum, should be calculated with a 95% confidence that 95% of the data lies above K_L . This is quantified by using the single-sided lower tolerance factors (U) provided in Table 2.1. For cases where more than 50 data samples are available, the tolerance factor equivalent to 50 samples can be used as a conservative number.

This method cannot be used to extrapolate the area of applicability beyond the limits of the validation data.

Table 2.1. Single-Sided Lower Tolerance Factors

# Experiments (n)	U
10	2.911
11	2.815
12	2.736
13	2.670
14	2.614
15	2.566
16	2.523
17	2.486
18	2.453
19	2.423
20	2.396
21	2.371
22	2.350
23	2.329
24	2.309
25	2.292
30	2.220
35	2.166
40	2.126
45	2.092
50	2.065

The one-sided lower tolerance limit is defined by the equation:

$$K_L = \bar{k}_{eff} - US_P \quad (20)$$

$$\text{If } \bar{k}_{eff} \geq 1, \text{ then } K_L = 1 - US_P \quad (21)$$

where:

$$\begin{aligned} S_P &= \text{square root (pooled variance)} \\ U &= \text{one-sided lower tolerance factor} \end{aligned}$$

Then:

$$USL = K_L - \Delta_{sm} - \Delta_{AOA} \quad (22)$$

and Δ_{sm} is the margin of subcriticality and Δ_{AOA} is an additional margin of subcriticality that may be necessary as a result of extensions to the area of applicability. If extensions are not made to the area of applicability, Δ_{AOA} is zero.

Tolerance Band

When a relationship between a calculated k_{eff} and an independent variable can be determined, a one-sided lower tolerance band may be used. This is a conservative method that provides a fitted curve above which the true population of k_{eff} is expected to lie. The tolerance band equation is actually a calibration curve relation. This was selected because it was anticipated that a given tolerance band would be used multiple times to predict bias. Other typical predictors such as a single future value, can only be used for a single future prediction to ensure the degree of confidence desired.

The equation for the one-sided lower tolerance band is

$$K_L = K_{fit}(x) - S_{P_{fit}} \left\{ \sqrt{2F_a^{(2,n-2)} \left[\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi_{1-\gamma, n-2}^2}} \right\} \quad (23)$$

$K_{fit}(x)$ is the function derived in the trend analysis described above. Because a positive bias may be nonconservative, the equation below must be used for all values of x where $K_{fit}(x) > 1$

$$K_L = 1 - S_{P_{fit}} \left\{ \sqrt{2F_a^{(2,n-2)} \left[\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi_{1-\gamma, n-2}^2}} \right\} \quad (24)$$

where:

$$\begin{aligned}
 p &= \text{the desired confidence (0.95)} \\
 F_{\alpha}^{(fit, n-2)} &= \text{the F distribution percentile with degree of fit, } n-2 \text{ degrees of freedom. The} \\
 &\quad \text{degree of fit is 2 for a linear fit. Note: The Excel® function is FINV(1-p, 2, n-2)} \\
 n &= \text{the number of critical experiment } k_{eff} \text{ values} \\
 x &= \text{the independent fit variable} \\
 x_i &= \text{the independent parameter in the data set corresponding to the "i"th } k_{eff} \text{ value} \\
 \bar{x} &= \text{the weighted mean of the independent variables} \\
 z_{2p-1} &= \text{the symmetric percentile of the Gaussian or normal distribution that contains the} \\
 &\quad \text{P fraction. Note: The Excel® function is NORMSINV(p)} \\
 \gamma &= \frac{1-p}{2} \\
 \chi_{1-\gamma, n-2}^2 &= \text{the upper Chi-square percentile Note: The Excel® function is} \\
 &\quad \text{CHIINV}(1-\gamma, n-2)
 \end{aligned} \tag{25}$$

It should be noted that some versions of Excel® are reported to erroneously compute certain statistical functions. Care should be taken to ensure that statistical functions are correctly calculated.

For a weighted analysis:

$$\sum (x_i - \bar{x})^2 = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} \tag{26}$$

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} \tag{27}$$

$$S_{P_R} = \sqrt{s_{fit}^2 + \bar{\sigma}^2} \tag{28}$$

where:

$$\bar{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} \tag{29}$$

and

$$s_{fit}^2 = \frac{\frac{1}{n-2} \sum \left\{ \frac{1}{\sigma_i^2} [k_{effi} - K_{fit}(x_i)]^2 \right\}}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} \tag{30}$$

Nonparametric Statistical Treatment

Data that do not follow a normal distribution can be analyzed by non-parametric techniques. The analysis results in a determination of the degree of confidence that a fraction of the true population of data lies above the smallest observed value. The more data available in the sample, the higher the degree of confidence.

The following equation determines the percent confidence that a fraction of the population is above the lowest observed value:

$$\beta = 1 - \sum_{j=0}^{m-1} \frac{n!}{j!(n-j)!} (1-q)^j q^{n-j} \quad (31)$$

where:

- q = the desired population fraction (normally 0.95)
- n = the number of data in one data sample
- m = the rank order indexing from the smallest sample to the largest (m = 1 for the smallest sample; m = 2 for the second smallest sample, etc.). Non-parametric techniques do not require reliance upon distributions, but are rather an analysis of ranks. Therefore, the samples are ranked from the smallest to the largest.

For a desired population fraction of 95% and a rank order of 1 (the smallest data sample), the equation reduces to:

$$\beta = 1 - q^n = 1 - 0.95^n \quad (32)$$

For example, if the number of data samples, $n = 19$, the $\beta = 62.3\%$, or there is a 62.3% confidence that 95% of the population lies above the smallest observed value. Notice that for fuel cycle facilities at least 59 critical experiments will need to be included in the validation in order to attain a 95% degree of confidence that 95% of the population lies above the smallest observed value. At this sample size the non-parametric margin is 0.

This information is then used to determine K_L , the combination of bias and bias uncertainty.

For non-parametric data analysis, K_L is determined by:

$$K_L = \text{Smallest } k_{\text{eff}} \text{ value} - \text{Uncertainty for Smallest } k_{\text{eff}} - \text{Non-parametric Margin (NPM)} \quad (33)$$

where:

NPM = Non-parametric margin. This non-parametric margin is added to account for small sample size and it is obtained from Table 2.2. The values in Table 2.2 are recommended values. Alternate values can be used with proper justification.

Smallest k_{eff} value = the lowest calculated value in the data sample.

If the smallest k_{eff} value is greater than 1, then the non-parametric K_L becomes:

$$K_L = 1 - S_p - \text{NPM} \quad (34)$$

where:

S_p = Square root of the pooled variance

Table 2.2. Non-Parametric Margins

Degree of Confidence for 95% of the Population	Non-parametric Margin (NPM)
>90%	0.0
>80%	0.01
>70%	0.02
>60%	0.03
>50%	0.04
>40%	0.05
≤40%	Additional data needed. (This corresponds to less than 10 data points.)

2.4.5 Identify and Support Subcritical Margin

As illustrated herein, determination of the USL relies on use of a subcritical margin to ensure that calculational results below that value of k_{eff} are adequately subcritical. The subcritical margin is not intended to account for process upset conditions or for uncertainties associated with a process. The subcritical margin is used solely to establish the maximum value of k_{eff} that can be considered to remain subcritical based on the validation results. The selection of the minimum subcritical margin to be used must be technically justified as part of the validation effort based on the systems to be modeled using the calculational method, the rigor of process controls to be applied, the reliability of the calculational method, and the knowledge of the physical and chemical aspects of the systems being modeled.

The value of minimum subcritical margin used to ensure subcriticality depends primarily upon the relative change in reactivity for a corresponding change in the process parameter being controlled for criticality safety (Winiarski and Risner, 1996). For some fissile systems, it requires a relatively large change in the process parameter to result in a significant change in the reactivity of the system. Provided that the parameter can be rigorously controlled, e.g., physical controls, then the use of a relatively small subcritical margin in k_{eff} is appropriate. However, the value of subcritical margin may need to be larger if reliance is placed on administrative controls for subcriticality. That is, the administrative controls can allow a variability in the parameter being controlled for criticality safety to have a disproportionately large reactivity effect. Sensitivity studies may be necessary to technically justify the ability to adequately control the parameter of interest to within a range of the parameter that assures only minor reactivity addition. In any case, the minimum subcritical margin, Δ_{SM} , must not be less than 0.02 in k_{eff} .

2.4.6 Calculation of Upper Safety Limit

The USL has been defined as follows:

$$USL = K_L - \Delta_{SM} - \Delta_{AOA} \quad (35)$$

Using this definition, a k_{eff} calculated by the code is required to meet the following condition to ensure subcriticality:

$$k_{\text{eff}} + 2\sigma_{\text{calc}} < \text{USL}, \quad (36)$$

where σ_{calc} is the statistical uncertainty calculated by the code.

2.5 DEFINE THE AREA OF APPLICABILITY OF THE VALIDATION AND LIMITATIONS

The area(s) of applicability refers to the key physical parameter(s) that define a particular fissile configuration. This configuration can either be an actual system or a process. The area of applicability refers to the breadth of a physical parameter associated with a series of experiments.

Use of practices described below will result in the following benefits:

- A consistent approach to determining the area of applicability,
- Standardized documentation of the area of applicability to determine if previously evaluated critical experiments can be used in bias determinations, and

The overall approach to develop and document the area of applicability of a system to be evaluated consists of the following steps:

1. Identifying the key parameters associated with the normal and upset conditions of the system to be evaluated.
2. From the key parameters identified above, establish a "screening" area of applicability for critical experiments.
3. Identify criticality experiments that are within this screening area of applicability or have the same key physical parameter.
4. From the scope of selected criticality experiments, determine the detailed area of applicability that the experiments cover.
5. Show that the system to be evaluated is within the area of applicability provided by the critical experiments or provide justification for using the critical experiment parameters for the system in question.
6. Document the results for the area of applicability.

Advanced techniques for establishing the area of applicability are under development at the Oak Ridge National Laboratory (Broadhead 1999).

Additional guidance on performing these steps is provided in the following sections.

Key physical parameters to be considered when defining the area of applicability fall into three categories: materials, geometry, and neutron energy spectrum. The parameters within these three areas are expanded in Table 2.3, and amplifying guidance is also provided. These values are derived by a number of experienced criticality safety specialists and are necessarily conservative in order for a consensus to be obtained. Alternative values can be used with appropriate justification.

Table 2.3. Physical Parameters for Areas of Applicability

Parameter	Critical Experiment Requirement ^{1,2}	Preferred Units of Measurement	Comment/Guidance																						
<u>MATERIALS</u> Fissionable Material	Validation experiments are to be of the same fissionable element(s) as the system(s) to be evaluated	N/A	One key purpose is to validate the cross-section library for the fissioning isotopes. Therefore, the fissioning isotopes must match.																						
Isotopic Composition	<div>For U-235, Pu-239, Pu-241:</div> <table><tr><td>Weight %</td><td>Allowable</td></tr><tr><td><u>(w/o)</u></td><td><u>Exp Range</u></td></tr><tr><td>0 - 2</td><td>± 1%</td></tr><tr><td>2 - 5</td><td>± 1.5%</td></tr><tr><td>5 - 10</td><td>± 2.5%</td></tr><tr><td>10 - 20</td><td>± 5%</td></tr><tr><td>20 - 80</td><td>± 15%</td></tr><tr><td>80 - 100</td><td>± 10%</td></tr></table> <div>For Pu-240:</div> <table><tr><td>Weight %</td><td>Allowable</td></tr><tr><td><u>(w/o)</u></td><td><u>Exp Range</u></td></tr><tr><td>0 - 32</td><td>± 4%</td></tr></table>	Weight %	Allowable	<u>(w/o)</u>	<u>Exp Range</u>	0 - 2	± 1%	2 - 5	± 1.5%	5 - 10	± 2.5%	10 - 20	± 5%	20 - 80	± 15%	80 - 100	± 10%	Weight %	Allowable	<u>(w/o)</u>	<u>Exp Range</u>	0 - 32	± 4%	weight percent	<p>The allowable experiment range gives the acceptable spread in weight percent of the specified isotope from the system to be evaluated (e.g., if the system is 90% U-235, experiments can range from 80% to 100%).</p> <p>Fissionable materials in quantities of less than 0.5% of total fissile material may be neglected.</p>
Weight %	Allowable																								
<u>(w/o)</u>	<u>Exp Range</u>																								
0 - 2	± 1%																								
2 - 5	± 1.5%																								
5 - 10	± 2.5%																								
10 - 20	± 5%																								
20 - 80	± 15%																								
80 - 100	± 10%																								
Weight %	Allowable																								
<u>(w/o)</u>	<u>Exp Range</u>																								
0 - 32	± 4%																								
Physical Form	Should be of same physical form (e.g., metal, solution, oxide, compound).	N/A	This may or may not always be achievable. If different physical forms, justification must be provided.																						
Concentration	No requirement	atom density	Experiments should be as close to the desired concentration as possible.																						
Temperature	<table><tr><td>Range</td><td>Tolerance</td></tr><tr><td>80 - 273°K</td><td>± 25°K</td></tr><tr><td>273 - 500°K</td><td>± 50°K</td></tr><tr><td>550 - 1100°K</td><td>± 100°K</td></tr></table>	Range	Tolerance	80 - 273°K	± 25°K	273 - 500°K	± 50°K	550 - 1100°K	± 100°K	degrees kelvin	<p>The temperature tolerances also apply to other materials (e.g., moderating, reflecting, and absorbing materials).</p> <p>Some cross section data in code libraries are temperature dependent. However, the range of temperatures is generally very broad.</p>														
Range	Tolerance																								
80 - 273°K	± 25°K																								
273 - 500°K	± 50°K																								
550 - 1100°K	± 100°K																								
<u>Moderation Material (in Fuel)</u>	Should be of the same moderating element(s) as system to be evaluated.	N/A	This may or may not always be achievable. If different moderators are used, justification must be provided.																						

Parameter	Critical Experiment Requirement ^{1,2}	Preferred Units of Measurement	Comment/Guidance
Isotopic Composition	For hydrogen, the composition should be within ± 20 atom% (a/o). For other element, no requirement.	atomic density	For in fuel moderation, the isotopic composition should be as close as possible. This is to validate the cross-section library at the expected neutron energy spectrum.
Physical Form	Should be same as system to be evaluated.	N/A	The physical form should be of the same chemical composition and phase.
Ratio to Fissile Material	Should be within $\pm 20\%$	Ratio of atom densities	
<u>Interstitial Moderation Material</u>	Should be the same moderating element(s) as system to be evaluated.	N/A	This may or may not always be achievable. If different moderators are used, justification must be provided.
Isotopic Composition	For hydrogen, the composition should be within ± 20 a/o. For other element, no requirement.	atomic density	
Physical Form	Should be same as system to be evaluated.	N/A	
Density	Within ± 10 w/o	weight percent	The density of the material is only one measure. The interstitial spacing for both normal and upset conditions of the system must also be considered.
<u>Reflector Material</u>	Should be same as system to be evaluated.	N/A	
Isotopic Composition	Within ± 10 w/o of system to be evaluated.	weight percent	
Physical Form	No requirement		
Density	Within $\pm 25\%$	grams/cc	
<u>Absorber Material</u>	Two classes: 1/v absorber (He-3, B-10, Li-6) – isotopes are interchangeable given the same macroscopic absorption at 2200 m/s. Other elements – should be the same elements.	N/A	This may or may not always be achievable. If different absorbers are used, justification must be provided and a larger subcritical margin may be warranted. Absorbers are nonfissionable, nonmoderative isotopes with microscopic absorption cross sections of greater than 2 barns at any energy. Non-1/v isotopes with macroscopic absorption cross sections of less than 10^4 cm^{-1} at any energy and an atom ratio with respect to the fissile material of less than 10^4 need not be considered.
Isotopic Composition	1/v isotopes – no addition restriction Other isotopes – the isotopic ratio should be within $\pm 5\%$.	N/A	
Physical Form	No restriction	N/A	
Ratio to Fissile Material	If the absorber is within the fuel, the atom ratio should be within 20%.	atom density	

Parameter	Critical Experiment Requirement ^{1,2}	Preferred Units of Measurement	Comment/Guidance
Density	If the absorber is in a reflector and the absorber contributes greater than 1% of the total absorption, then the atom ratio of absorber/scatterer and absorber/fissionable (if applicable) should be within 20%.	atom density	
<u>Geometry</u>	This section is common to both homogeneous and heterogeneous systems. For additional guidance, see LA-12683, Appendix E.		The geometry should be as close as possible to the actual case. Geometry is not considered as important as material specifications.
Shape	For non-reentrant bodies, $\pm 50\%$ variation on mean cord length For internal reentrant bodies, $\pm 25\%$ variation on mean cord length. For external reentrant bodies, no tolerance in shape or size	mean cord length	Mean chord length is calculated as: $4 * \text{volume/surface area}$ The shape can impact the cross-section determination in the code. For example, SCALE uses three types of calculation that are dependent on shape and size: inhommedium, lattice cell, and multiregion.
Reflection	Solid angle to within $\pm 10\%$. Mean spacing between reflector and fuel within $\pm 10\%$.	N/A	
Relative material thickness	Physical thickness of all materials should agree within $\pm 50\%$.		
<u>Neutron Energy</u>	The neutron energy spectra is to cover the same energy range, e.g., thermal (0 - .1 eV), intermediate (1 - 100 KeV), or fast (100 KeV - 20 MeV).		The cross section libraries are neutron energy dependent, so ensuring the experiments fall within the right energy range is important to validation.

¹From tolerance limits specified in LA-12683, Appendix E. Ranges are for interpolation purposes.

²For information on extrapolation ranges, refer to Section 5.

Identifying and Evaluating Analysis Parameters

The first step in performing a validation is to identify the range of parameters for which the validation will apply. Critical experiments should be selected that span the range of parameters. This initially defines the areas of applicability for the validation. An iterative process is required to finally establish the area of applicability. The number of available critical experiments and the results of the statistical evaluation may necessitate some changes to the boundaries of the area(s) of applicability. It may also be necessary to increase the margin of subcriticality where there are relatively few critical experiments. When initially determining the range of parameters for the validation, consideration should be given to the needs of subsequent analyses that will evaluate both normal and credible upset conditions.

Identifying Applicable Critical Experiments

After the system parameters have been identified, a target area of applicability can be formulated using Table 2.3. This area serves as initial screening criteria for selecting critical experiments. Experiments which are proposed for validation in the area of applicability should be compared against these screening criteria. Use of experiments outside the identified area of applicability should be justified.

Determining Area of Applicability of Critical Experiments

Once the experiments have been selected, then the areas of applicability can be quantified (or identified) for each experiment. The collective data can then be used to form the area of applicability for each parameter. The analyst needs to consider the overall parametric span and try to ensure that experiments provide a spectrum of critical experiments throughout the range. For example; if the H/X ratio ranges from 0 to 5000 for the experiments, and there are no experiments covering the majority of the range (i.e., the experiments tend to be at the extreme ends of the range), then the ability to interpolate inside the range is questionable. It may be desirable to include additional critical experiments in the validation. Often experiments within these ranges do not exist or are not readily available. In such cases, a larger margin of subcriticality will be needed.

Guidance for extrapolation in LA-12683 gives typical extrapolation ranges for the parameters presented in Table 2.3. These values are provided for information. Should extrapolation of critical experiments area of applicability be required, justification should be documented. Margin will be affected by extrapolation as described in Section 5.

Comparing Range of Evaluated System to Range of Critical Experiments

Once the detailed area of applicability for the experiments has been determined, a point by point comparison of parameters should be performed against the system to be evaluated. Table 2.4 provides an example of the development of an Area of Applicability Table and this point by point comparison. In this example MIT fuel is compared against the pertinent parameters for SPERT D fuel critical experiments. For important parameters, the experimental range should be shown to cover, or be within the extrapolation ranges of the system of interest. The purpose of defining the area of applicability is to verify that the neutron physics will not be unduly affected by parameters not accounted for in experiments. If important parameters are found to be greatly outside the experimental range, other methods, such as sensitivity studies, are required as discussed in Section 5.

Calculations made for actual criticality safety analyses should not use code options (e.g., albedo, biasing, boundary conditions, etc.) that are dissimilar from those used in the validation. These code options incorporate approximations of the code response. Unless these options are also validated their use is not appropriate.

Documentation of Area of Applicability

After the areas of applicability are determined, the evaluation process needs to be properly documented. The documentation consists of the items below:

- **Area of Applicability Table** – used to document the detailed evaluation.
- **Discussion of Less Important Parameters** – used to provide amplifying information (if applicable) of parameters considered but determined to be less important for validation.

Area of Applicability Table

The area of applicability table contains the detailed information gathered during the determination process (See Table 2.4). It contains the key parameters for:

- The system to be evaluated,
- Each set of critical experiments selected,
- The area of applicability covered by the critical experiments, and
- Validation comments.

The validation comments for each parameter identify if the area of applicability of the critical experiments covers the system to be evaluated.

Discussion of Less Important Parameters

During the course of the evaluation, many physical parameters of the actual system may be found to be inconsequential for validation purposes. For example, a fuel storage pool made of concrete may contain sufficient water surrounding the fuel to consider the system to be water reflected, with concrete having little or no impact on the neutron physics. For this case, concrete need not be considered as a reflecting material.

Table 2.4. Example Area of Applicability Table

This section of the documentation would identify such items and their exclusionary basis to retain the knowledge in the evaluation process. This eliminates future questions on the thoroughness of the review.

It may also be useful to provide a summary of the area of applicability in the introduction or abstract of the validation reports and/or calculations. The summary should address the characteristics described in Table 2.5.

Table 2.5. Items Contained in the Area of Applicability Summary

Characteristic	Comment
Fissile Material	Specify the type of fuel and enrichment.
Moderation	Identify moderating materials and if possible, quantify a measure of moderation (e.g., H/X ratio). Interstitial moderation may be characterized by thickness of moderator.
Reflection	Identify the reflecting materials and associated thickness (if applicable).
Absorption	Identify the absorbing materials and associated thickness (if applicable).
Neutron Energy Spectrum	Identify the average energy group range or the neutron energy range.

2.6 FORMALIZING THE VALIDATION REPORT

The validation activity must be documented in a formal report. The report must have sufficient detail to allow for independent review by qualified individuals. This report should describe the methodology for determining the USL and areas of applicability for the code system. The validation report must address the activities and information described below. The format for the written validation report is presented in Section 6.

The validation report should provide a summary description of the facility or site for which the validation is to apply, including details relevant to NCS (i.e., fissile isotope(s), enrichment, chemical compounds, density ranges of fissile material, moderators, reflectors, etc.). There should also be a description of the computer code system used, applicable code execution sequences, cross section libraries, and the computer system for which the validation is performed. If the validation is to be used for multiple workstations or personal computers of the same type, then each computer's unique designation is to be listed along with an indication, on a machine-by-machine basis, of the area of applicability for which the code system is valid. The list of machines for which the validation is applicable may be maintained separate from the formal validation report if the response from each machine is essentially identical. The list should be kept current. A change in the list does not imply a need to revise the validation report if all systems have the same bias, bias uncertainty, and applied USL.

For each area of applicability, each critical experiment used to determine the bias and associated bias uncertainty for that area of applicability will be listed in the validation report. Each critical experiment should be given a unique identifier, a summary description, and justification on the appropriateness of that experiment for the intended area of applicability. The source of the critical experiment along with a citation where more details can be found is to be cited or included in the report. Methods for preparation of basic data (i.e., H/X determination) and constants used should either be described or citations provided where such descriptions exist.

The input files used in the validation should be included. When reporting the results, notations should be provided for unusual or unexpected results. Tables should be provided of calculated k_{eff} values and uncertainty by critical experiment designation, with applicable independent parameters, grouped by area of applicability. The calculated k_{eff} values and uncertainties should be provided in a graphical as well as a tabular manner. A clear statement or table of areas of applicability should be provided.

The statistical methods used in the determination of the USL should be described or a citation provided where such descriptions exist. The results of calculations for bias, bias uncertainty, bias trending, hypothesis testing for normality (or other distribution), subcritical margin, and derivation of the USL should be provided. Sufficient detail should be provided to facilitate review and checking of the calculation by a qualified individual. The means for determining and demonstrating the area of applicability should be discussed. If the USL varies as a function of some independent parameter, a graphical depiction should be provided of the USL function with the calculated k_{eff} values. If an area of applicability is extended to cover a range of a parameter that is outside the validation data, then the detailed calculations and technical basis to support the extension must be provided.

Finally, a comprehensive list of references used in the validation should be provided of sources of critical experiment data, statistical methods employed, and other relevant information. An input listing for each critical experiment modeled in the format of the code system being validated should be provided. Parametric sensitivity calculations should have at least one input listing provided with a clear indication of the parameter(s) varied.

3. SAMPLE DETERMINATION OF BIAS AND BIAS UNCERTAINTY

Following are a set of sample calculations to illustrate the methodologies described in Section 2. The data in Table 3.1 below is used in the calculations. The H/X ratio is used as the independent parameter for this example

Table 3.1. Sample Data

H/X	k_{eff}	σ_{calc}	σ_{exp}	σ_t^*
421.8	0.9848	0.0014	0.0049	0.0051
421.8	0.9869	0.0015	0.0049	0.0051
421.8	0.9864	0.0013	0.0049	0.0051
195.2	0.9990	0.0015	0.0049	0.0051
195.2	0.9961	0.0015	0.0049	0.0051
293.9	1.0004	0.0018	0.0049	0.0052
293.9	0.9963	0.0014	0.0049	0.0051
406.3	0.9964	0.0015	0.0049	0.0051
495.9	0.9969	0.0018	0.0049	0.0052
613.6	0.9927	0.0013	0.0049	0.0051
613.6	0.9921	0.0016	0.0049	0.0052
971.7	0.9881	0.0013	0.0049	0.0051
971.7	0.9856	0.0015	0.0049	0.0051
133.4	1.0039	0.0016	0.0049	0.0052
133.4	1.0114	0.0018	0.0049	0.0052
133.4	1.0108	0.0017	0.0049	0.0052
133.4	1.0071	0.0018	0.0049	0.0052
133.4	1.0064	0.0022	0.0049	0.0054
133.4	1.0113	0.0018	0.0049	0.0052
133.4	1.0128	0.0021	0.0049	0.0053
133.4	1.0067	0.0018	0.0049	0.0052
276.9	1.0054	0.0018	0.0049	0.0052
276.9	1.0053	0.0016	0.0049	0.0052
276.9	1.0071	0.0020	0.0049	0.0053
276.9	1.0112	0.0019	0.0049	0.0053

*The column labeled σ_t is found by the application of equation (3), $\sigma_t = \sqrt{\sigma_{calc}^2 + \sigma_{exp}^2}$.

Throughout this example numbers have been truncated to show only significant digits, however to avoid roundoff error it is prudent to retain as many significant digits as possible for intermediate calculations and truncate the final result to those digits which may be considered significant.

This set of calculations has been performed for a 95% confidence level.

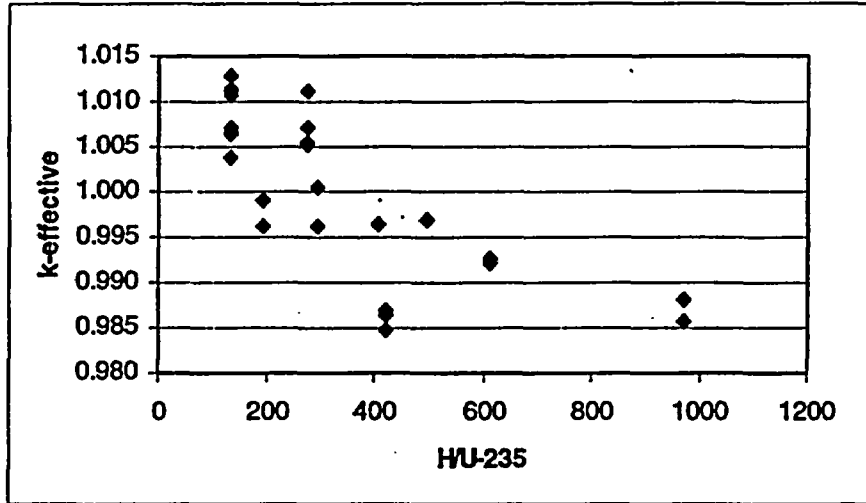


Figure 3.1. Input Critical Experiment Data

From Figure 3.1 the data appears well distributed and a trend in the data is somewhat apparent. It appears that the calculated k_{eff} values increase as moderation (H/U-235 ratio) decreases.

The first thing to do is calculate the weight for each k_{eff} value. The weight is calculated from equation (3).

Utilizing the equations in Table 2.1, it is necessary to determine the variance about the mean, average total uncertainty, and the weighted mean k_{eff} value. There are 25 k_{eff} values in our data set, therefore $n=25$. The k_{eff} value is represented by "y" in the variance about the mean (s^2) equation.

The weighted mean k_{eff} value is found by application of equation (6):

$$\bar{k}_{eff} = \frac{\sum \frac{1}{\sigma_i^2} k_{eff,i}}{\sum \frac{1}{\sigma_i^2}} = 0.99983$$

The variance about the mean is found from equation (4):

$$s^2 = \frac{\frac{1}{(n-1)} \sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} = 8.47993 \times 10^{-5}$$

The average total uncertainty is found from equation (5):

$$\overline{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} = 2.67991 \times 10^{-5}$$

The square root of the pooled variance, from equation (7):

$$S_p = \sqrt{s^2 + \overline{\sigma}^2} = 1.056 \times 10^{-2}$$

Therefore, for the single-sided tolerance limit method the bias is equal to $k_{\text{eff}} - 1 = -1.659 \times 10^{-4}$ with an associated uncertainty of 1.056×10^{-2} .

The next goal is to identify trends in the data, and determine the model coefficients for the weighted linear fit of the data, $y(x) = a + bx$.

Applying equations (11), (12), and (13);

$$\Delta = \sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2} \right)^2 = 4.949 \times 10^{16}$$

$$a = \frac{1}{\Delta} \left(\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i^2}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} \right) = 1.00967$$

$$b = \frac{1}{\Delta} \left(\sum \frac{1}{\sigma_i^2} \sum \frac{x_i y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} \right) = -2.863 \times 10^{-5}$$

The weighted linear model for k_{eff} as a function of H/U-235 using equation (10) is therefore

$$K_{\text{fit}}(x) = 1.00967 - 2.863 \times 10^{-5} x.$$

It is evident upon review of the equation that at low H/U-235 ratios the value of k_{eff} will exceed 1. Where $K_{\text{fit}}(x) > 1$, it is necessary to assign a value of 1. For this case, that point corresponds to H/U-235 less than 337.8.

Goodness of Fit

The linear-correlation coefficient is determined using equation (14).

$$r = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\left[\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2 \right]} \sqrt{\left[\sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2 \right]}}$$

In order to evaluate this equation it is necessary to determine the weighted mean of the independent variable, x , which in this case is the weighted mean of the H/U-235 ratio. From equation (15):

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} = 343.58$$

From previous calculation, the weighted mean $\bar{k}_{eff} \equiv \bar{y} = 0.99983$.

$$\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2 = 5.31 \times 10^{10}$$

$$\sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2 = 75.9423$$

$$\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})(y_i - \bar{y}) = -1.52 \times 10^6$$

$$r = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\left[\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2 \right]} \sqrt{\left[\sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2 \right]}} = -0.76$$

$$r^2 = 0.57$$

Shapiro-Wilk Test for Normality

In order for a Tolerance Limit approach to be used it must be demonstrated that the data is normally distributed. The Shapiro-Wilk Test requires the calculation of several statistical terms. The maximum number of terms " v " is calculated by $(n-1)/2$ if n is odd and $n/2$ if n is even. Since n for this example is 25 experiments, $v=12$. The multiplication constant (α_j) is taken from Appendix A as a function of n and j , the index. For this example, the values are taken from the column corresponding to $n=25$, with j values 1 - 12. These are provided in Table A.2.

Prior to this point within this example " x_i " has represented the H/U-235 ratio. The Shapiro-Wilk Test does not require the use of an independent variable. The term \bar{y} refers to the standard unweighted average of k_{eff} and y_i are the " i^{th} " k_{eff} values. For this example the average k_{eff} is 1.000044. The weighted average value of k_{eff} can also be used and may be more desirable if elsewhere weighted values are used.

The mechanics of the calculation require the analyst to place the k_{eff} values in ascending order, indexing them from 1 to n .

$$Y = \sum_{j=1}^v \alpha_j (y_{(n+1-j)} - y_j) = 4.3147 \times 10^{-2}$$

$$S^2 = \sum (y_i - \bar{y})^2 = 2.0276 \times 10^{-3}$$

$$W_r = \frac{Y^2}{S^2} = 0.9182$$

From Table A.5 for $n=25$ a percentage point of 0.918 is extracted. If W_r , the test statistic, is greater than 0.918 then it can be said that this set of values is normally distributed. This set passes - marginally. Therefore, it is appropriate to perform a single sided tolerance limit for this set of k_{eff} values.

If weighted average is used for \bar{y} (i.e., $\bar{y} = \bar{k}_{eff} = 0.99983$), then S^2 is 2.0287×10^{-3} and W_r becomes 0.9177. This value is slightly below the cut-off value for a normal distribution.

4. SAMPLE DETERMINATION OF UPPER SAFETY LIMIT

Single Sided Tolerance Limit and USL Example

As previously demonstrated, the bias uncertainty for this set of critical experiment k_{eff} values is 0.01056 and the weighted mean k_{eff} is 0.99983. From Table 2.1, "Single Sided Lower Tolerance Factors," yields a value of $U = 2.292$ for an n of 25. Thus, applying equation (20),

$$K_L = \bar{k}_{eff} - US_P = 0.97562.$$

If the mean k_{eff} had exceeded 1, then a value of 1 would have been assigned to the mean k_{eff} value. The USL adds additional margin for extending the AOA and a safety margin. The safety margin is a margin that separates the maximum k_{eff} of a modeled configuration from a potentially critical configuration. The area of applicability margin is based on sensitivity studies and engineering judgement and is used to apply a model whose k_{eff} data do not appropriately represent the physical parameters of the model. If a value of 0.02 is assigned to the safety margin, Δ_{sm} , and the AOA margin, Δ_{AOA} , is determined to be 0.03, then the Upper Safety Limit is calculated as shown in equation (22).

$$USL = K_L - \Delta_{sm} - \Delta_{AOA} = 0.92562$$

The Upper Safety Limit (USL) and K_L are shown in Figure 4.1, in relation to the k_{eff} calculations.

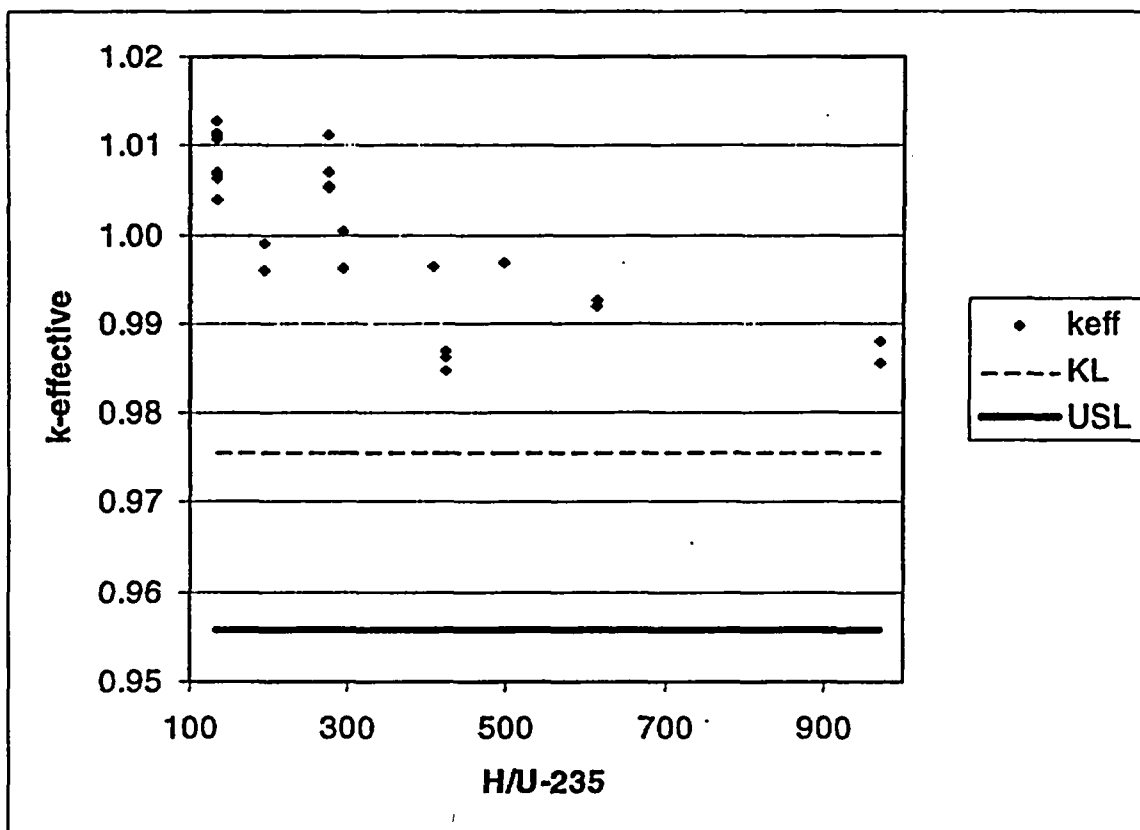


Figure 4.1. K_L and USL

Non-Parametric Statistical Treatment

If the data had failed the test for normality, a non-parametric treatment of the data would be necessary. It is assumed that the k_{eff} dataset failed the normality test. There are 25 data points, $n=25$. This example will be performed for a 0.95 population fraction (q). Therefore, from equation (32),

$$\beta = 1 - q^n = 1 - 0.95^{25} = 72.26\%.$$

Table 2.2 states that for values of β greater than 70% a non-parametric margin of 0.02 is appropriate.

This non-parametric subcritical margin will be applied to the smallest k_{eff} value in the k_{eff} set and the error associated with that value. The smallest k_{eff} value in this set is 0.9848 with a calculation error ($\sigma_{s,j}$) of 0.0014 and an experiment error ($\sigma_{e,j}$) of 0.0049. The proper interpretation of the statistical treatment is that there is a 72.26 % confidence that 95% of the population lies above the smallest observed value of 0.9848 minus the uncertainty for that value. The uncertainty is 0.0051.

Therefore, from equation (33),

$$K_L = \text{smallest } k_{eff} - \text{uncertainty for smallest } k_{eff} - \text{Non-parametric Margin (NPM)} = 0.9597$$

If the smallest k_{eff} had been greater than 1 then the equation (34)

$$K_L = 1 - S_p - \text{NPM}$$

would have been the appropriate form to use.

Keeping the same Δ_{SM} and Δ_{AOA} used in the Tolerance Limit example;

$$USL = K_L - \Delta_{sm} - \Delta_{AOA} = 0.9097$$

Single Sided Tolerance Band - Weighted Linear Example

This method requires the use of several statistical terms. The F distribution percentile can be extracted from an EXCEL® function, FINV(0.05,2,(n - 2)), for $\alpha=0.05$, P or $\beta=0.95$ (95% confidence level). The "2" indicates that this is a linear fit, and $F_{\alpha}^{(fit,n-2)} = 3.422$. The "symmetrical percentile of the Gaussian or Normal distribution that contains the P fraction," $Z_{2P,1}$, can be extracted from the EXCEL® function NORMSINV(0.95), for the 95% confidence level and is 1.645. The upper Chi-square percentile, χ^2 , requires an input $\gamma=1-\alpha/2-\beta=0.025$ for a 95% confidence level. The EXCEL® function, CHIINV(1- γ , n-2) or CHIINV(0.975,23), yields the desired input for this calculation with $n=25$, $\chi^2=11.689$.

The equation previously derived for the weighted linear model is:

$$K_{fit}(x) = 1.00967 - 2.863 \times 10^{-5} x.$$

Using equations (28), (29), and (30)

$$S_{p,s} = \sqrt{s_{fit}^2 + \bar{\sigma}^2}$$

where

$$\bar{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} = 2.68 \times 10^{-5}$$

where the weight is the same value previously used in this example and n is 25.

and

$$s_{fit}^2 = \frac{\frac{1}{(n-2)} \sum \left\{ \frac{1}{\sigma_i^2} [k_{eff_i} - k_{fit}(x_i)]^2 \right\}}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} = 3.782 \times 10^{-5}$$

$$S_{P_{\mu}} = \sqrt{s_{fit}^2 + \bar{\sigma}^2} = 0.008039$$

For this weighted linear model the weighted mean is used for the equation of K_L .

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}}$$

Restating the equation, all of the required components are now known and the value of K_L can be calculated for each point. Assuming that the Δ_{SM} is 0.02, the USL is determined by subtracting 0.02 from the K_L . For $K_{fit}(x)$ values greater than 1, $K_{fit}(x)=1$. From equation (23)

$$K_L = K_{fit}(x) - S_{P_{\mu}} \left\{ \sqrt{2F_{\alpha}^{(2,n-2)} \left[\frac{1}{n} + \frac{(x - \bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi_{1-\gamma, n-2}^2}} \right\}$$

For a weighted problem the term, equation (26)

$$\sum (x_i - \bar{x})^2 = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}}$$

Tabular results from the application of these equations for the sample problem are shown in Table 4.1. Graphical results are shown in Figure 4.2.

Table 4.1. Calculation of the Tolerance Band and USL Values

x	y _i	$k_{fit(x)}$ or 1 (if $k_{fit(x)} > 1$)	K_L	USL
421.8	0.9848	0.9976	0.9746	0.9546
421.8	0.9869	0.9976	0.9746	0.9546
421.8	0.9864	0.9976	0.9746	0.9546
195.2	0.9990	1.0000	0.9765	0.9565
195.2	0.9961	1.0000	0.9765	0.9565
293.9	1.0004	1.0000	0.9772	0.9572
293.9	0.9963	1.0000	0.9772	0.9572
406.3	0.9964	0.9980	0.9751	0.9551
495.9	0.9969	0.9955	0.9719	0.9519
613.6	0.9927	0.9921	0.9672	0.9472
613.6	0.9921	0.9921	0.9672	0.9472
971.7	0.9881	0.9819	0.9515	0.9315
971.7	0.9856	0.9819	0.9515	0.9315
133.4	1.0039	1.0000	0.9758	0.9558
133.4	1.0114	1.0000	0.9758	0.9558
133.4	1.0108	1.0000	0.9758	0.9558
133.4	1.0071	1.0000	0.9758	0.9558
133.4	1.0064	1.0000	0.9758	0.9558
133.4	1.0113	1.0000	0.9758	0.9558
133.4	1.0128	1.0000	0.9758	0.9558
133.4	1.0067	1.0000	0.9758	0.9558
276.9	1.0054	1.0000	0.9771	0.9571
276.9	1.0053	1.0000	0.9771	0.9571
276.9	1.0071	1.0000	0.9771	0.9571
276.9	1.0112	1.0000	0.9771	0.9571

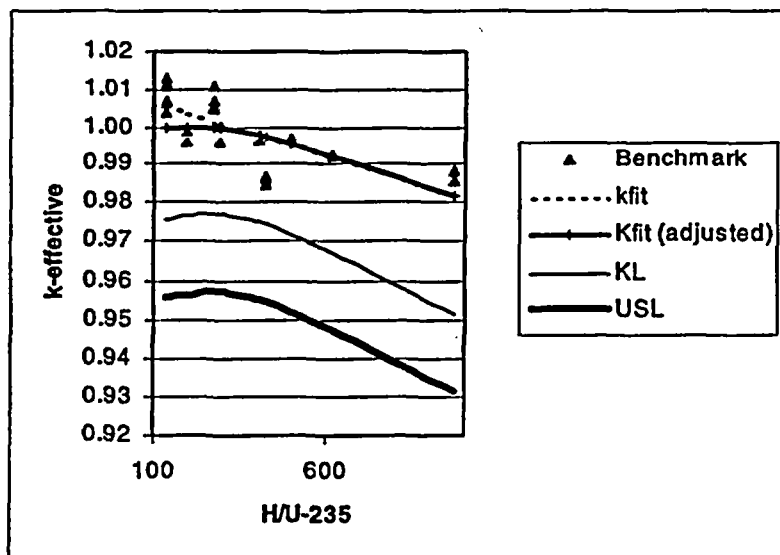


Figure 4.2. Linear Weighted Tolerance Band Example

5. EXTENDING THE AREA OF APPLICABILITY

When preparing a process analysis it is necessary to compare bounding calculated k_{eff} values with the USL in order to establish safety limits. Such calculations must be performed within the area of applicability for the validation study specific to the computer system and code used. If a material or parameter for the system being analyzed is outside the area of applicability, then the analyst must either revise the validation using critical experiments that provide a suitable area of applicability for the system or justify an extension to the area of applicability. Extension of the area of applicability should be supported by sensitivity studies in which only the parameter(s) being extrapolated is varied to identify trends in the bias.

For example, the critical experiments are for uranium oxyfluoride solutions but the system being analyzed is uranyl nitrate. A sensitivity study with calculations using both uranium oxyfluoride solutions and uranyl nitrate solutions can be used to determine the relative sensitivity of k_{eff} to the solution diluent. Extension of the area of applicability may require an additional margin of subcriticality to account for increased uncertainty in the bias results due to extrapolation of the validation results. Determination of this additional margin, Δ_{AOA} , should be based on the results of the sensitivity study (bias trends) as well as engineering judgement. Using this additional margin, the USL for the code becomes:

$$USL = K_L - \Delta_{SM} - \Delta_{AOA} \quad (21)$$

Depending on the statistical technique used to establish the USL, the margin due to extension of the area of applicability may already be accounted for in the determination of bias. For example, use of the tolerance band (described in Section 2.4.4) and confidence band techniques accounts for uncertainty in extrapolation of the quantified parameters. Using these techniques, the bias uncertainty increases when the tolerance or confidence bands are extrapolated beyond the validation data. Thus, no additional margin may be necessary to account for extension of the area of applicability when applying these techniques. Caution should be exercised, however, since use of the tolerance limit technique does not allow direct extrapolation of the parameters beyond the limits of the validation data.

The ANSI/ANS-8.1 standard requires supplementation of the calculational method if the extrapolation is large. In general, if the extrapolation is larger than 10 percent from the validation data, then the validation should be revised to include additional critical experiments to enhance the area of applicability. Similarly, if there are large regions in the values of a parameter over which there is no validation data, then the validation should also be supplemented to include additional critical experiment data in this range. More specific guidance for ranges of extrapolation for particular parameters is provided in Table 2.3. It may not always be safe to extrapolate to the extent provided by this guidance. The data should be carefully examined prior to this extrapolation. In the absence of suitable critical experiments, a detailed technical basis must be provided. The basis must support the methods used for extending the area of applicability and identify the techniques for determination of the USL and additional margin to account for the increased bias uncertainty.

6. SAMPLE FORMAT FOR LICENSEE VALIDATION REPORTS

Section 2.6 describes specific information that should be included in the written validation report. Following is a recommended general format for validation reports that provides a consistent approach to documenting the validation analysis and results. Each of these sections should be included in the written report as appropriate.

Title/Signature Page

The validation report should be uniquely identified and be signed by the primary author(s) and the person conducting the independent technical or peer review.

Introduction

This section should provide a brief introduction to the validation by stating what is being validated, the calculational method being used, and the systems to be evaluated using the validation results.

Calculational Method or Code System

The calculational method or code system being validated should be described, including the major software modules, data sets used in the validation, hardware, and other pertinent information.

Validation Methodology

This section should describe the approach and techniques used to perform the validation, including the statistical method used, the area of applicability based on the systems to be evaluated, the basis for the subcritical margin used, and other appropriate information.

Critical Experiment Descriptions

A description of the critical experiments used in conducting the validation should be presented along with a discussion of the source of the data and grouping of experiments based on the parameters of interest.

Analysis of Validation Results

This section should provide the analysis of the validation results. This includes the results of the calculations, trending analysis, the detailed statistical analysis (including the basis for acceptability of the statistical technique chosen), calculation of the bias, bias uncertainty, the area of applicability, the USL for each distinct area of applicability of the parameters of interest, and the technical basis for any extensions of the areas of applicability.

Conclusions

A compilation of the validation results should be provided in this section, including the detailed description of the areas of applicability, the USL to be used for each area of applicability, and the results and limitations for any extensions of the areas of applicability.

7. BIBLIOGRAPHY

American National Standards Institute/American Nuclear Society, "Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry," ANSI/ANS-10.4-1987, May 1987.

American National Standards Institute/American Nuclear Society, "Nuclear Criticality Safety in Operations With Fissionable Material Outside Reactors," ANSI/ANS-8.1-1998, September 1998.

American Society of Mechanical Engineers, "Quality Assurance Requirements of Computer Software for Nuclear Facility Applications," ASME NQA-2a-1990, Part 2.7, 1990.

Bethea, R.M., Duran, B.S., and Boullion, T.L., "Statistical Methods for Engineers and Scientists", Decker, 1995.

Bevington, P.H., "Data Reduction and Error Analysis for the Physical Sciences," McGraw-Hill Book Company, New York, 1969.

Bowen, M.W., and Bennett, C.A., "Statistical Methods for Nuclear Material Management," NUREG/CR-4604, PNL-5849, Pacific Northwest National Laboratory, December 1988.

Bredehoft, B.B., and Busch, R.D., "Characterization of the Thermalness of a Fissile System With a Two-Group Diffusion Theory Parameter," Nuclear Technology, Vol. 102, pp. 259-269, May 1993.

Broadhead, B.L., Childs, R.L., and Rearden, B.T., "Computational Methods for Sensitivity and Uncertainty Analysis in Criticality Safety," Oak Ridge National Laboratory, presented to the ICNC '99 Sixth International Conference on Nuclear Criticality Safety, September 20-24, 1999, Versailles, France.

Broadhead, B.L., Hopper, C.M., and Parks, C.V., "Proposed Methodology for Establishing Area of Applicability," Oak Ridge National Laboratory, presented to the ICNC '99 Sixth International Conference on Nuclear Criticality Safety, September 20-24, 1999, Versailles, France.

Carter, R.D., "Problems in Validating Criticality Safety Calculations," RHO-HS-SA-70 P, Rockwell Hanford Operations, June 1985.

Carter, R.D., "Validating Calculations for Criticality Safety," Y/DD-521, Vol. I, Oak Ridge Y-12 Plant, April 1993.

Crawford, C., and Palmer, B.M., "Validation of MCNP, A Comparison With SCALE. Part 1: Highly Enriched Uranium Solutions," WINCO-1109, Idaho National Engineering Laboratory, October 1992.

Crawford, C., and Palmer, B.M., "Validation of MCNP, A Comparison With SCALE. Part 2: Highly Enriched Uranium Metal Systems," WINCO-1110, Idaho National Engineering Laboratory, October 1992.

Crawford, C., and Palmer, B.M., "Validation of MCNP, A Comparison With SCALE. Part 3: Highly Enriched Uranium Oxide Systems," WINCO-1111, Idaho National Engineering Laboratory, October 1992.

Crawford, C., and Palmer, B.M., "Validation of MCNP: SPERT-D and BORAX-V Fuel," WINCO-1112, Idaho National Engineering Laboratory, November 1992.

D'Agostino, R.B., and Stephens, M.A., "Goodness-of-Fit Techniques," Marcel Dekker, Inc., New York, 1986.

DeHart, M.D., and Bowman, S.M., "Validation of the SCALE Broad Structure 44-Group ENDF/B-V Cross-Section Library for Use in Criticality Safety Analyses," NUREG/CR-6102, ORNL/TM-12460, Oak Ridge National Laboratory, July 1994.

Disney, K., "A Review of the Current State-of-the-Art Methodology for Handling Bias and Uncertainty in Performing Criticality Safety Evaluations," INEL-94/0251, Idaho National Engineering Laboratory, October 1994.

Dyer, H.R., Jordan, W.C., and Cain, V.R., "A Technique for Code Validation for Criticality Safety Calculations," Transactions of the American Nuclear Society, Vol. 63, pp. 238-239, June 1991.

Dyer, H.R. and Parks, C.V., "Recommendations for Preparing the Criticality Safety Evaluation of Transportation Packages", NUREG/CR-5661, ORNL/TM-11936, Oak Ridge National Laboratory, April 1997

Emmett, M.B., and Jordan, W.C., "Guide to Verification and Validation of the SCALE-4 Criticality Safety Software," NUREG/CR-6483, ORNL/TM-12834, Oak Ridge National Laboratory, November 1996.

Harmon, C.D. II, Busch, R.D., Briesmeister, J.F., and Forster, R.A., "Criticality Calculations with MCNP: A Primer," LA-12827-M, Los Alamos National Laboratory, August 1994.

Hopper, C.M., "Validation of Computational Methods and Data for Nuclear Criticality Safety Applications," Oak Ridge National Laboratory (see <http://tis.eh.doe.gov/criticality/> for information), February 1999.

Jordan, W.C., "Validation of SCALE 4.0—CSAS25 Module and the 27-Group ENDF/B-IV Cross-Section Library for Low-Enriched Uranium Systems," ORNL/CSD/TM-287, Oak Ridge National Laboratory, February 1993.

Jordan, W.C., Landers, N.F., and Petrie, L.M., "Validation of KENO V: A Comparison with Critical Experiments," ORNL/CSD/TM-238, Oak Ridge National Laboratory, December 1986

Lichtenwalter, J.J., Bowman, S.M., DeHart, M.D., and Hopper, C.M., "Criticality Benchmark Guide for Light-Water-Reactor Fuel in Transportation and Storage Packages", NUREG/CR-6361, ORNL/TM-13211, Oak Ridge National Laboratory, March 1997.

Morey, D.C., and Damon, D.R., "Validation Practices in the United States," U.S. Nuclear Regulatory Commission, submitted to the ICNC '99 Sixth International Conference on Nuclear Criticality Safety, September 20-24, 1999, Versailles, France.

Nomura, Y., and Shimooke, T., "A Multiple Regression Equation for Calculated k_{eff} Bias Errors by Criticality Code System," *Nuclear Technology*, Vol. 65, pp. 340-349, May 1984.

Nuclear Energy Agency, "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NCS/DOC(95)03, Nuclear Energy Agency, Organization for Economic Co-Operation and Development, September 1998.

Press, W.H., et al, "Numerical Recipes in Fortran - The Art of Scientific Computing," 2nd Ed., Cambridge Press, 1992.

Rutherford, D., "Forecast of Criticality Experiments and Experimental Programs Needed to Support Nuclear Operations in the United States of America: 1994-1999," LA-12683, Los Alamos National Laboratory, reissued July 1994.

Sitaraman, S., "MCNP: Light Water Reactor Critical Benchmarks," NEDO-32028, Class I, General Electric Nuclear Energy, March 1992.

Transport Methods Group, "MCNP4XS Monte Carlo N-Particle Transport Code System," Los Alamos National Laboratory, October 1998, Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-663, July 1999.

Transport Methods Group, "MCNP4XS Standard Neutron, Photon, and Electron Data Libraries for MCNP4XS," Los Alamos National Laboratory, January 1997, Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as DLC-198B, January 1999.

Trumble, E.F., and Kimball, K.D., "Statistical Methods for Accurately Determining Criticality Code Bias," DE97060128, presented at 1997 conference Criticality Safety Challenges in the Next Decade at Lake Chelan, Washington, CONF-970926-11, September 1997.

U.S. Nuclear Regulatory Commission, "Nuclear Criticality Safety Standards for Fuels and Material Facilities," Regulatory Guide 3.71, January 1998.

U.S. Nuclear Regulatory Commission, "SCALE, A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation," NUREG/CR-0200, Rev. 4 (ORNL/NUREG/CSD-2/R4), Vols. I-III (April 1995). Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

Wagner, J.C., Sisolak, J.E., and McKinney, G.W., "MCNP: Criticality Safety Benchmark Problems," LA-12415, Los Alamos National Laboratory, October 1992.

Westinghouse Savannah River Company, "Nuclear Criticality Safety Methods Manual," WSRC-IM-96-133, Rev. 0, September 1996.

Winiarski, R. Jr., and Risner, V., "Analysis of the Sensitivity of Calculated k_{eff} to Changes in NCS Parameters," *Transactions of the American Nuclear Society*, Vol. 74, p. 217, Reno, Nevada, June 1996.

APPENDIX A. TABLES USED FOR SHAPIRO-WILK NORMALITY TEST

Table A.1. Shapiro-Wilk Test Normality Test Coefficients—10–20 Samples

I	N										
	10	11	12	13	14	15	16	17	18	19	20
1	0.5739	0.5601	0.5475	0.5359	0.5251	0.5150	0.5056	0.4968	0.4886	0.4808	0.4734
2	0.3291	0.3315	0.3325	0.3325	0.3318	0.3306	0.3290	0.3273	0.3253	0.3232	0.3211
3	0.3141	0.2260	0.2347	0.2412	0.2460	0.2495	0.2521	0.2540	0.2553	0.2561	0.2565
4	0.1224	0.1429	0.1586	0.1707	0.1802	0.1878	0.1939	0.1988	0.2027	0.2059	0.2085
5	0.0399	0.0695	0.0922	0.1099	0.1240	0.1353	0.1447	0.1524	0.1587	0.1641	0.1686
6		0.0000	0.0303	0.0539	0.0727	0.0880	0.1005	0.1109	0.1197	0.1271	0.1334
7				0.0000	0.0240	0.0433	0.0593	0.0725	0.0837	0.0932	0.1013
8							0.0196	0.0359	0.0496	0.0612	0.0711
9								0.0000	0.0163	0.0303	0.0422
10										0.0000	0.0140

Table A.2. Shapiro-Wilk Test Normality Test Coefficients—21–30 Samples

I	N									
	21	22	23	24	25	26	27	28	29	30
1	0.4643	0.4590	0.4542	0.4493	0.4450	0.4407	0.4366	0.4328	0.4291	0.4254
2	0.3185	0.3156	0.3126	0.3098	0.3069	0.3043	0.3018	0.2992	0.2968	0.2944
3	0.2578	0.2571	0.2563	0.2554	0.2543	0.2533	0.2522	0.2510	0.2499	0.2487
4	0.2119	0.2131	0.2139	0.2145	0.2148	0.2151	0.2152	0.2151	0.2150	0.2148
5	0.1736	0.1764	0.1787	0.1807	0.1822	0.1836	0.1848	0.1857	0.1864	0.1870
6	0.1399	0.1443	0.1480	0.1512	0.1539	0.1563	0.1584	0.1601	0.1616	0.1630
7	0.1092	0.1150	0.1201	0.1245	0.1283	0.1316	0.1346	0.1372	0.1395	0.1415
8	0.0804	0.0878	0.0941	0.0997	0.1046	0.1089	0.1128	0.1162	0.1192	0.1219
9	0.0530	0.0618	0.0696	0.0764	0.0823	0.0876	0.0923	0.0965	0.1002	0.1036
10	0.0263	0.0368	0.0459	0.0539	0.0610	0.0672	0.0728	0.0778	0.0822	0.0862
11	0.0000	0.0122	0.0228	0.0321	0.0403	0.0476	0.0540	0.0598	0.0650	0.0697
12			0.0000	0.0107	0.0200	0.0284	0.0358	0.0424	0.0483	0.0537
13					0.0000	0.0094	0.0178	0.0253	0.0320	0.0381
14							0.0000	0.0084	0.0159	0.0227
15									0.0000	0.0076

Table A.3. Shapiro-Wilk Test Normality Test Coefficients—31–40 Samples

I	N									
	31	32	33	34	35	36	37	38	39	40
1	0.4220	0.4188	0.4156	0.4127	0.4096	0.4068	0.4040	0.4015	0.3989	0.3964
2	0.2921	0.2898	0.2876	0.2854	0.2834	0.2813	0.2794	0.2774	0.2755	0.2737
3	0.2475	0.2463	0.2451	0.2439	0.2427	0.2415	0.2403	0.2391	0.2380	0.2368
4	0.2145	0.2141	0.2137	0.2132	0.2127	0.2121	0.2116	0.2110	0.2104	0.2098
5	0.1874	0.1878	0.1880	0.1882	0.1883	0.1883	0.1883	0.1881	0.1880	0.1878
6	0.1641	0.1651	0.1660	0.1667	0.1673	0.1678	0.1683	0.1686	0.1689	0.1691
7	0.1433	0.1449	0.1463	0.1475	0.1487	0.1496	0.1505	0.1513	0.1520	0.1526
8	0.1243	0.1265	0.1284	0.1301	0.1317	0.1331	0.1344	0.1356	0.1366	0.1376
9	0.1066	0.1093	0.1118	0.1140	0.1160	0.1179	0.1196	0.1211	0.1225	0.1237
10	0.0899	0.0931	0.0961	0.0988	0.1013	0.1036	0.1056	0.1075	0.1092	0.1108
11	0.0739	0.0777	0.0812	0.0812	0.0873	0.0900	0.0924	0.0947	0.0967	0.0986
12	0.0585	0.0629	0.0669	0.0669	0.0739	0.0770	0.0798	0.0824	0.0848	0.0870
13	0.0435	0.0485	0.0530	0.0530	0.0610	0.0645	0.0677	0.0706	0.0733	0.0759
14	0.0289	0.0344	0.0395	0.0395	0.0484	0.0523	0.0559	0.0592	0.0622	0.0651
15	0.0144	0.0206	0.0262	0.0262	0.0361	0.0404	0.0444	0.0481	0.0515	0.0546
16	0.0000	0.0068	0.0131	0.0131	0.0239	0.0287	0.0331	0.0372	0.0409	0.0444
17			0.0000	0.0000	0.0119	0.0172	0.0220	0.0264	0.0305	0.0343
18					0.0000	0.0057	0.0110	0.0158	0.0203	0.0244
19							0.0000	0.0053	0.0101	0.0146
20									0.0000	0.0049

Table A.4. Shapiro-Wilk Test Normality Test Coefficients—41–50 Samples

I	N									
	41	42	43	44	45	46	47	48	49	50
1	0.3940	0.3197	0.3894	0.3872	0.3850	0.3830	0.3808	0.3789	0.3770	0.3751
2	0.2719	0.2701	0.2684	0.2667	0.2651	0.2635	0.2620	0.2604	0.2589	0.2574
3	0.2357	0.2345	0.2334	0.2323	0.2313	0.2302	0.2291	0.2281	0.2271	0.2260
4	0.2091	0.2085	0.2078	0.2072	0.2065	0.2058	0.2052	0.2045	0.2038	0.2032
5	0.1876	0.1874	0.1871	0.1868	0.1865	0.1862	0.1859	0.1855	0.1851	0.1847
6	0.1693	0.1694	0.1695	0.1695	0.1695	0.1695	0.1695	0.1693	0.1692	0.1691
7	0.1531	0.1535	0.1539	0.1542	0.1545	0.1548	0.1550	0.1551	0.1553	0.1554
8	0.1385	0.1392	0.1398	0.1405	0.1410	0.1415	0.1420	0.1423	0.1427	0.1430
9	0.1249	0.1259	0.1269	0.1278	0.1286	0.1293	0.1300	0.1306	0.1312	0.1317
10	0.1123	0.1136	0.1149	0.1160	0.1170	0.1180	0.1189	0.1197	0.1205	0.1212
11	0.1004	0.1020	0.1035	0.1049	0.1062	0.1073	0.1085	0.1095	0.1105	0.1113
12	0.0891	0.0909	0.0927	0.0943	0.0959	0.0972	0.0986	0.0998	0.1010	0.1020
13	0.0782	0.0804	0.0824	0.0842	0.0860	0.0876	0.0892	0.0906	0.0919	0.0932
14	0.0677	0.0701	0.0724	0.0745	0.0765	0.0783	0.0801	0.0817	0.0832	0.0846
15	0.0575	0.0602	0.0628	0.0651	0.0673	0.0694	0.0713	0.0731	0.0748	0.0764
16	0.0476	0.0506	0.0534	0.0560	0.0584	0.0607	0.0628	0.0648	0.0667	0.0685
17	0.0379	0.0411	0.0442	0.0471	0.0497	0.0522	0.0546	0.0568	0.0588	0.0608
18	0.0283	0.0318	0.0352	0.0383	0.0412	0.0439	0.0465	0.0489	0.0511	0.0532
19	0.0188	0.0227	0.0263	0.0296	0.0328	0.0357	0.0385	0.0411	0.0436	0.0459
20	0.0094	0.0136	0.0175	0.0211	0.0245	0.0277	0.0307	0.0335	0.0361	0.0386
21	0.0000	0.0045	0.0087	0.0126	0.0163	0.0297	0.0229	0.0259	0.0288	0.0314
22			0.0000	0.0042	0.0081	0.0188	0.0153	0.0185	0.0215	0.0244
23					0.0000	0.0039	0.0076	0.0111	0.0143	0.0174
24							0.0000	0.0037	0.0071	0.0104
25									0.0000	0.0035

Table A.5. Percentage Points For The W Test for Normality

N	W	N	W
10	0.842	31	0.929
11	0.850	32	0.930
12	0.859	33	0.931
13	0.866	34	0.933
14	0.874	35	0.934
15	0.881	36	0.935
16	0.887	37	0.936
17	0.892	38	0.938
18	0.897	39	0.939
19	0.901	40	0.940
20	0.905	41	0.941
21	0.908	42	0.942
22	0.911	43	0.943
23	0.914	44	0.944
24	0.916	45	0.945
25	0.918	46	0.945
26	0.920	47	0.946
27	0.923	48	0.947
28	0.924	49	0.947
29	0.926	50	0.947
30	0.927		

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11. ABSTRACT (200 words or less)

Evaluations for nuclear criticality safety must assure that subcritical conditions are present under both normal and credible off-normal conditions. Such evaluations typically rely upon computational techniques that are capable of modeling complex three-dimensional systems. An upper safety limit (USL) must be established based on a documented validation, under which acceptable calculated neutron multiplication or keef values must fall to be considered subcritical. The USL is established through the statistical evaluation of the calculational bias. The bias is the difference between critical experimental conditions similar to the area of applicability of interest and the calculated results of those experiments. This report describes procedures by which nuclear fuel cycle facility licensees may perform the validation activity, including determination of calculational bias, bias uncertainty, and an USL. Also included are suggested topics for inclusion in formal documentation of the validation activity.

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